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SHAPE OPTIMIZATION USING THE LEAST SQUARES METHOD

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ABSTRACT

SHAPE OPTIMIZATION
USING THE LEAST-SQUARES METHOD
by Edward E. Nelson

Historically, shape optimization has been performed by nesting the partial differential equations (PDEs) analysis within the optimization problem. A new procedure to perform shape optimization by simultaneously solving the governing PDEs and the optimum shape using the least-squares discrete point method has been developed. The proposed method treats this nested problem as a large single optimization problem by simultaneously solving the PDEs and minimizing the objective shape functions. Finite element shape functions were used to approximate the governing differential equations with the response variables (such as displacements) and the structural parameters being the design variables. The C_{m-1} continuity requirement was overcome by reducing the governing differential equations to an equivalent system of first-order differential equations. Mesh distortion and remeshing have been eliminated by allowing the mesh to remain stationary while the boundary moves relative to it. The fillet shape problem was optimized and compared with published results.

ACKNOWLEDGMENTS

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CHAPTER 1

Introduction

One of the goals of structural design is to obtain a feasible design while minimizing some function such as weight, volume, or area. Current optimization methods solve the analysis problem for each design iteration. The proposed method uses finite element shape functions to approximate the governing PDEs and simultaneously solves for the optimum shape parameters using the least-squares discrete point method. The discrete least squares approach requires only the location of the points on the boundary where the boundary conditions should be satisfied. The boundary can be defined by any set of points and does not need to include element nodes. The only requirement is that the boundary be inside the domain of the approximating functions and elements. With this new method the boundary can move anywhere inside the element mesh, thereby eliminating any need to remesh the model with each shape change.

Review of Least Squares Methods

The literature on the solution of differential equations by least squares is spread over many disciplines, so the review was narrowed to include only boundary value problems using the discrete point method of weighted residuals and the least squares finite element formulation.

Stress analysis has been performed using least squares for many linear and non-linear problems[1,2,3,4,5]. These solutions have been shown to be comparable and many times superior to the finite difference or finite element methods[6]. The discrete point method[7] used in this study is a general purpose technique which solves the interior and boundary equations at discrete points. The differential equations are evaluated at discrete points by solving for the undetermined parameters in the approximating functions. The error in solving the differential equations at each point is called the residual error. The parameters in the approximating function that minimize the sum of the square of the residual errors are found using a non-linear least squares technique. This method is simple and allows the use of a large class of approximating functions. Hulbert and Niedenfuhr used this method to solve the complicated problem of finding the stress concentrations in a thin plate with multiple circular and noncircular holes. They used Aires stress formulation combined with Howland functions to construct the stress functions for each set of holes. These functions were evaluated at the interior and boundary nodes and their residuals minimized to get the final solution. The least squares solution was very accurate having a maximum error less than 0.1%.

When the variational function does not exist it is possible to obtain a standard finite element formulation by applying the weighted residuals principle to the governing differential equations. This method called the discrete least squares finite element method, was developed by Lynn and Arya[8]. It has been used successfully by numerous authors[9,10] to solve solids, fluids, and heat transfer problems. In this method the nodal variables are the unknowns and the residual errors from the differential equations are evaluated for each element, and integrated over the elements area. These element integrals are then assembled into a global matrix similar to the finite element stiffness matrix. This method like the finite element method gives a symmetric matrix from which the unknown nodal quantities can be determined.

Review of Shape Optimization Methods

Shape optimization has developed as the computers became faster, so most of the literature has been written in the last ten years. This literature covers various penalty functions, conjugate gradient methods and linear programming techniques for minimizing the objective functions. All of these methods require some sensitivity analysis that provides the rate of change of the response variable (e.g. stress and displacements) with respect to changes in the design variables. Sensitivity analysis involves taking the derivatives of some function with respect to the design variables. These partial derivatives can then be used to estimate the response of a revised design to a specified perturbation without having to reanalyze the problem. The basic approach is to obtain an initial solution and then calculate the sensitivity derivatives either analytically or numerically. The sensitivity derivatives show which of the design variables have the most effect on the response to design changes. Using this information a new design is chosen which further minimizes the objective functions. This process is repeated until the design converges to an acceptable solution. The new shape, even though similar to the initial shape will be different. As the elements distort their shape functions lose the ability to approximate the solution of the PDE problem. This distortion of the finite element mesh causes inaccuracies in the calculation of stresses and displacements as well as their sensitivity derivatives. It is therefore necessary to use an adaptive mesh refinement scheme based on error estimates[11], or use a different analysis model based on higher order polynomials[12,13]. The primary methods for calculating the sensitivity derivatives are the implicit differentiation method[14] and the material derivative method. In the implicit derivative method the finite element stiffness matrix is numerically differentiated with respect to the design variables, usually by the finite difference method. This requires access to the element stiffness matrix, which is not usually possible with commercial finite element codes. This method has been shown to be very sensitive to round-off errors in the numerical differentiation. The second method uses the material derivative of continuum mechanics on an elastic body. The material derivative is a dynamic mapping of the deformation and involves calculating the velocity field. The expressions for the sensitivity derivatives are now continuous functions which are evaluated using the boundary element or finite element methods. Using the sensitivity information the design variables are changed to get an improved shape which is then discretized and reanalyzed completing one iteration of the optimization process. This process, shown in Figure 1, is continued until the design has converged to an acceptable solution.

There has been some work done in simultaneous analysis and design methods[15] using the conjugate gradient method. For these studies the thickness and cross sectional areas were optimized while the actual shape was held fixed. This method was shown to be accurate and efficient when compared with other iterative methods.

Conclusions

The traditional method of shape optimization is an iterative process, with the analysis being nested inside the design optimization. It requires remeshing of the model, as the boundary must be defined by the element nodes in the finite element method. By using the discrete point least square method and working with the governing differential equations the boundary may now move within the element during optimization. This allows the optimization and analysis parts to be solved simultaneously.

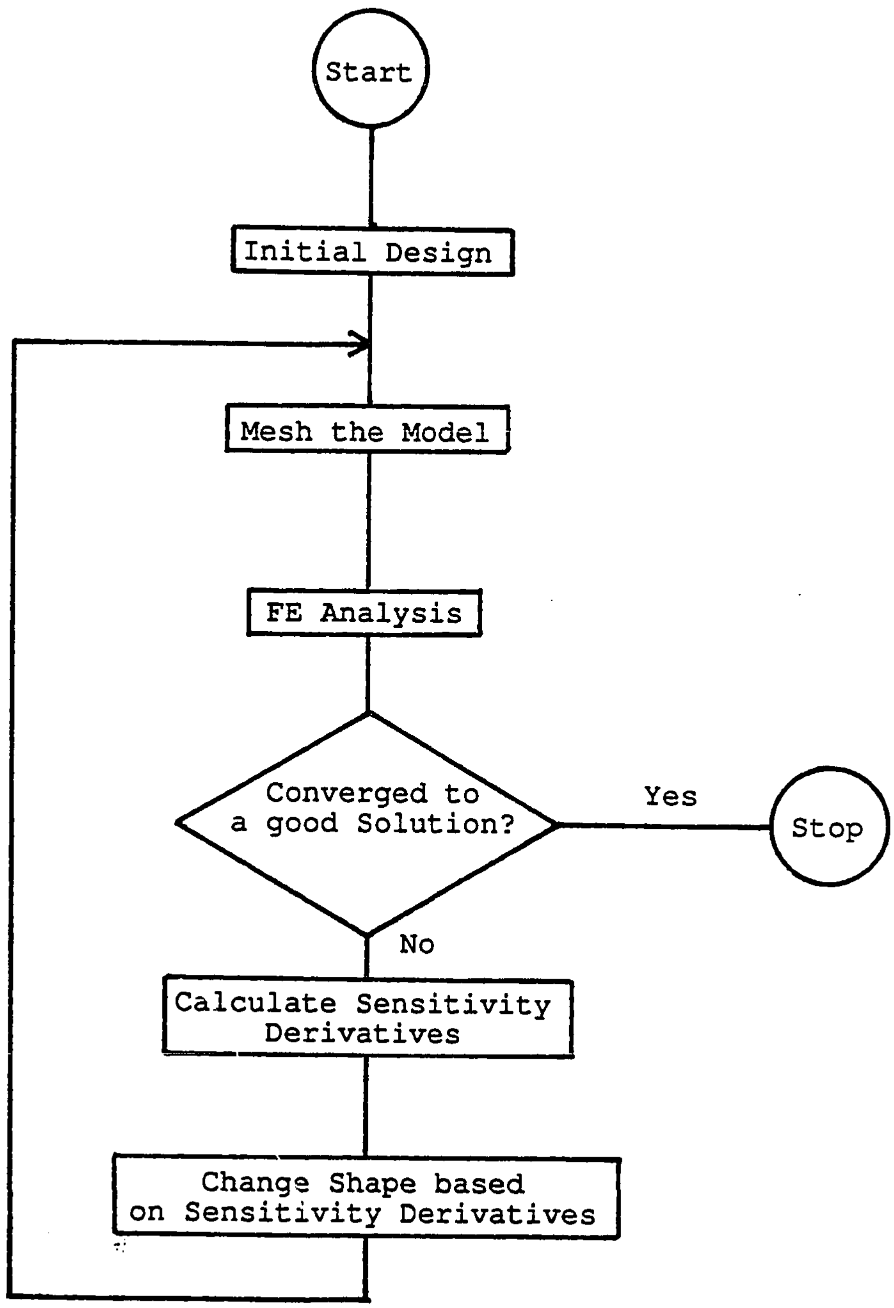

Figure 1 Method of solution for a typical shape optimization problem

CHAPTER 2

Differential Equation Approach

There are two general methods for solving the mechanics of deformable bodies problems. One is the finite element method which uses the variational energy principle, which transforms the problem into one of finding the minimum of the energy functional. This method only works on problems for which the variational principles exist. The second method involves solving the governing differential equations which represent the behavior of an infinitesimal element in the body, and forcing the solution match the boundary conditions. The differential equation can then be solved numerically using various methods such as the finite difference method or the method of weighted residuals.

The method of weighted residual is a technique for obtaining solutions to linear and nonlinear partial differential equations. The first step is to assume the general functional form of the solution for the field variable. The assumed form should approximately satisfy the differential equations and boundary equations. This trial solution, usually a polynomial with undetermined coefficients is then substituted into the governing differential equations and boundary equations and evaluated at discrete points, where it generates a residual error for each point. The residual error is then minimized over the entire solution domain by minimizing the integral of the square of the residual errors with respect to the undetermined coefficients.

By minimizing the error residuals over the entire domain, the coefficients of the approximating trial function can be determined and also the solution of the problem.

By using the governing differential equations you gain versatility; however, major difficulties arise in the construction of admissible element trial functions that conform to the inter-element continuity requirements. It has been shown[16] that if in the governing differential equation the highest derivative of the unknown function is *m*, then its *(m-1)* derivative must be continuous across element boundaries. Since the higher order derivatives usually appear in the differential equations, higher order element approximating functions are required. However, this constraint can be avoided by uncoupling the differential equation into an equivalent system of lower order equations and adding inter-element continuity constraints.

Discrete Point Least Squares Formulation

The discrete least squares method is a general purpose method for solving both linear and nonlinear PDE problems. Least squares always produces a positive definite matrix and can be shown to produce uniform convergence, in many cases with pointwise error bounds[17]. The least squares method will be described for the following boundary value problem. Let the physical boundary value problem be described by the governing differential equation

$$L_m(\Phi) = f \qquad (2\text{-}1)$$

in domain D subject to the boundary condition

$$B(\phi)=g \tag{2-2}$$

on the boundary. Where L_m denotes the differential operator with highest order m, ϕ is the unknown function, f and g are functions, and B is the differential boundary operator. The object is to find a solution ϕ^* that results in a minimum residual error when substituted into equations 2-1 and 2-2. A trial solution ϕ^* which can be represented by

$$\phi^*(a,x,y)\approx\phi(x,y) \tag{2-3}$$

where a is the solution vector with n unknown parameters (nodal variables in this study), and x, y represent the independent variables of the domain. The trial solution is then substituted into the above equations, which generate the residuals

$$R_D=L_m(\phi^*)-f \tag{2-4}$$

in the domain D and

$$R_B=B(\phi^*)-g \tag{2-5}$$

on the boundary. Where R_D and R_B are called interior and boundary residuals, respectively. The domain D is subdivided into k regions or elements, and the trial function ϕ^* is defined as a sum of the element trial functions or shape functions

$$\phi^*=\sum_{i=1}^{k}\phi_i^* \tag{2-6}$$

where the subscript i denotes the i^{th} element. An approximate solution is for ϕ^* is then substituted into equations 2-1,2 which generate the following residuals r

$$\begin{pmatrix} r_1(a) \\ \cdot \\ \cdot \\ r_k(a) \\ r_{k+1}(a) \\ \cdot \\ \cdot \\ r_m(a) \end{pmatrix} = \begin{pmatrix} L_m(\phi^*(a,x_1,y_1))-f \\ \cdot \\ \cdot \\ L_m(\phi^*(a,x_k,y_k))-f \\ W_1B(\phi^*(a,x_j,y_j))-g \\ \cdot \\ \cdot \\ W_pG(\phi^*(a,x_p,yp))-g \end{pmatrix} \tag{2-7}$$

A residual is calculated for every point and inter-element continuity residuals are calculated at the midside of the element boundaries, as ϕ^* is locally defined. The weight W_i represents weighting of the boundary residuals relative to the interior residuals. The residuals r are calculated for each a using Powell's non-linear least square method[18]. Powell's method was selected because the analytical derivatives of r with respect to a are not required. This method iteratively searches for the minimum sum of squares, r^Tr, along directions determined by solving the gauss equations for generalized least squares. This method is efficient because the inverse matrix is updated rather than being computed at each iteration.

<u>Triangular Finite Element Approximating Function</u>

The mathematical interpretation of the finite element requires us to view the element as a part of the solution domain where the phenomena of interest are occurring. Once the solution domain has been modeled by the finite element mesh, the behavior of the field variable and its derivatives behavior is approximated by continuous functions expressed in terms of the nodal values. These functions defined over each element are called interpolation functions or shape functions. The collection of interpolation functions for the whole solution domain provides a piecewise approximation of the field variable. To guarantee monotonic convergence of the approximate solution to the correct solution certain requirements for the interpolating functions must be met:

1) $C_{(m-1)}$ Continuity- At the element boundaries the field variable and any of its partial derivatives up to one order less than the highest order $(m-1)$ derivative appearing in the governing equation must be continuous.
2) Completeness- All uniform states of u and its derivatives up to the m^{th} order of the governing equation must be included in u. This requires a complete polynomial of order m as a minimum element expansion.

The flat triangular element has been extensively used as a basic finite element, because an assemblage of such elements can approximate not only arbitrary planar regions, but also free form curved surfaces. The element chosen was a four node triangular element, shown in Figure 2, with ten degrees of freedom, three (u, $\partial u/\partial x$, $\partial u/\partial y$) at each corner node and one, u, at the center node. This ten degree of freedom element uses a 3^{rd} order polynomial for the approximating function, which gives a cubic variation of displacement and quadratic variation of strain. The element shape functions are[19]

$$\phi=\left(\phi_1,\frac{\partial\phi_1}{\partial x},\frac{\partial\phi_1}{\partial y},\phi_2,,,\frac{\partial\phi_3}{\partial y},\phi_4\right)\begin{pmatrix} L_1^2(3-2L_1)-7L_1L_2L_3 \\ L_1^2(x_{21}L_2-x_{13}L_3)+(x_{13}-x_{21})L_1L_2L_3 \\ L_1^2(y_{21}L_2-y_{13}L_3)+(y_{13}-y_{21})L_1L_2L_3 \\ \vdots \\ 27L_1L_2L_3 \end{pmatrix}$$

where $x_{ij}=x_i-x_j$, $y_{ij}=y_i-y_j$
L_1, L_2, L_3 *are local area coordinates*

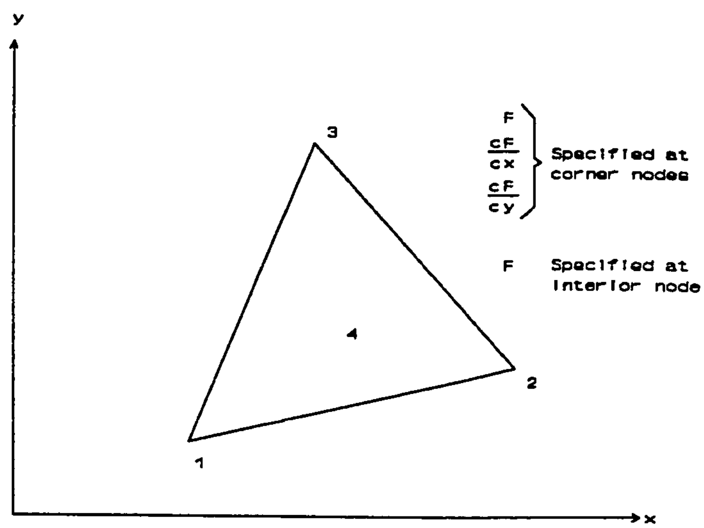

Figure 2 Triangular element with a cubic interpolation function.

The strain variation is not continuous across element boundaries as it is specified by two nodal values when three are required for continuity. The continuity requirement for strain can be approximately enforced by making a least squares residual at each element boundary midpoint and minimizing the error of the differences of the strains. Basically the object is to approximate strain continuity for the element by requiring the nodal unknowns to minimize the error in strain at a point at the middle of the element boundary, as shown in Figure 3. This effectively gives the needed extra strain point to ensure inter-element continuity for strain.

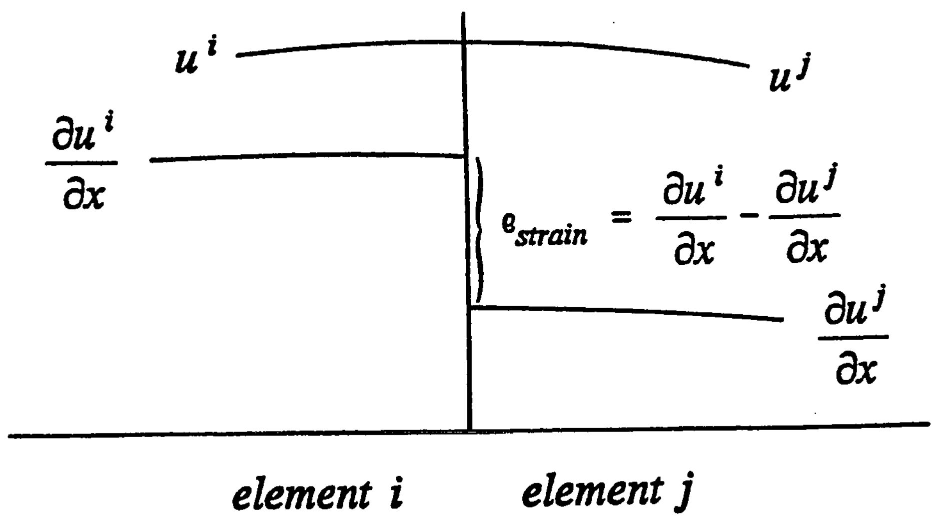

Figure 3 Description of the error residual for strain at the element midside.

Governing Equations and Material Relationships

The Equilibrium equations and material relationships characterize the state of a point in an elastic body. The plane strain equilibrium equations in standard form are

$$\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + \frac{1}{1-2\nu}\ \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + X = 0 \tag{2-8}$$

$$\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + \frac{1}{1-2\nu}\ \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + Y = 0 \tag{2-9}$$

where u and v are the displacements in the x and y directions, respectively, and X and Y are the body forces. The plane strain material relationships between stress and strain, as governed by Hooke's law are

$$\sigma_{xx} = \frac{E}{(1+\nu)(1-2\nu)}\left((1-\nu)\epsilon_{xx} + \nu\epsilon_{yy}\right) \tag{2-10}$$

$$\sigma_{yy} = \frac{E}{(1+\nu)(1-2\nu)}\left((1-\nu)\epsilon_{yy} = \nu\epsilon_{xx}\right) \tag{2-11}$$

$$\sigma_{zz} = \frac{E}{(1+\nu)(1-2\nu)}\left(\epsilon_{xx} + \epsilon_{yy}\right) \tag{2-12}$$

$$\sigma_{xy} = \frac{E}{(1+\nu)}\ \epsilon_{xy} \tag{2-13}$$

$$\sigma_{xz} = \sigma_{yz} = 0 \tag{2-14}$$

where ε_{xx} and ε_{yy} are the normal strains in the x and y directions, ε_{xy} is the sheer strain, E is Young's modulus, and ν is Poisson's ratio. The strain displacement relationships are

$$\epsilon_{xx} = \frac{\partial u}{\partial x} \tag{2-15}$$

$$\epsilon_{yy} = \frac{\partial v}{\partial y} \tag{2-16}$$

$$\epsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \tag{2-17}$$

$$\epsilon_{zz} = \epsilon_{xz} = \epsilon_{yz} = 0 \tag{2-18}$$

The compatibility equations are

$$\frac{\partial^2 \epsilon_{xx}}{\partial x^2} + \frac{\partial^2 \epsilon_{yy}}{\partial x^2} = \frac{\partial^2 \epsilon_{xy}}{\partial x \partial y} \tag{2-19}$$

By selecting displacements as the field variable the compatibility equations are automatically satisfied and need not be considered. On the Boundary when nodal values of stress or displacement are known these replace unknown values reducing the total DOF of the problem. Along boundaries between nodes the stress boundary condition is

$$T_x = \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)l + \mu\,[2\frac{\partial u}{\partial x}l + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)m] \tag{2-20}$$

$$T_y = \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)m + \mu\,[2\frac{\partial v}{\partial y} + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)l\ ] \tag{2-21}$$

where l and m are the direction cosines of the normal vector, Tx and Ty are the components of the stress vector, λ and μ are the Lamé constants. The two equilibrium equations are calculated at the four interior Gauss points in every element.

Uncoupled Differential Equations

The continuity constraint can be relaxed by uncoupling the governing differential equation into an equivalent set of first order differential equations. We may replace equation 2-8,9 by a set of equivalent first order partial differential equations

$$\frac{\partial u}{\partial x} - \zeta = 0 \qquad (2\text{-}22)$$

$$\frac{\partial u}{\partial y} - \zeta^{*} = 0 \qquad (2\text{-}23)$$

$$\frac{\partial v}{\partial x} - \eta = 0 \qquad (2\text{-}24)$$

$$\frac{\partial v}{\partial y} - \eta^{*} = 0 \qquad (2\text{-}25)$$

$$\left(\frac{\partial \zeta}{\partial x} + \frac{\partial \zeta^{*}}{\partial y}\right) + \frac{1}{1-2\nu}\,\frac{\partial}{\partial x}(\zeta + \eta^{*}) = 0 \qquad (2\text{-}26)$$

$$\left(\frac{\partial \eta}{\partial x} + \frac{\partial \eta^{*}}{\partial y}\right) + \frac{1}{1-2\nu}\,\frac{\partial}{\partial y}(\zeta + \eta^{*}) \qquad (2\text{-}27)$$

where ζ, ζ^{*}, η, and η^{*} are unknown auxiliary functions. Equations 2-22 through 2-27, now require C_0 continuity.

Design Optimization Methodology

A new and innovative way to do shape optimization has been found that moves the boundary within the finite element shape functions while the boundary nodes remaining stationary. There is no problem with mesh distortion or its resulting inaccuracies. This is the key factor for allowing the simultaneous solution method to succeed. Without having to remesh before each analysis step, the least squares code can solve for the optimum shape and the field variables simultaneously, with the optimum shape being the shape that best minimizes the objective functions.

The boundary is defined by a function, such as an ellipse or a cubic spline, that is fully defined by the design variables. The design variables need to be constrained such that the boundary will always be within the model element mesh. This is done by applying a parabolic error whenever the design variables violate this constraint. This error is calculated as the square of the distance from the legitimate solution space. The more the constraint is violated the larger the error becomes.

In order for this method to work, the boundary conditions must be met along the surface as it moves through the element. The nodes outside the surface have no physical meaning, they are just needed to approximate the governing differential equations and the trial functions inside the body. Equilibrium residuals are not calculated at any of the element interior points that lie outside of the body, as shown in Figure 4. It is therefore necessary to calculate equilibrium on the moving boundary so as to provide enough equations to uniquely determine the nodal unknowns that fall outside of the body.

Least squares needs an objective function to minimize with respect to the shape. These functions can be weight, area, volume, displacements, or any other appropriate functions. The two objective functions used in this work are area and maximum tangential stress on the body. The area under a fillet was to be minimized with the constraint that the maximum tangential stress could not exceed the yield strength. A parabolic error residual was added when the maximum stress exceeded yield to force the desired solution.

Moving the boundary in the elements is a valid way to simultaneously do the analysis and optimization. This is possible as remeshing is not required prior to analysis with each design change. An intricate boundary can be modeled by relatively simple functions that require only a few design variables. This means that the optimization will increase the total degree of freedom of the problem by just a few degrees. As many analysis models contain hundreds or thousands of DOF's, the addition of a few more for the design variables is insignificant.

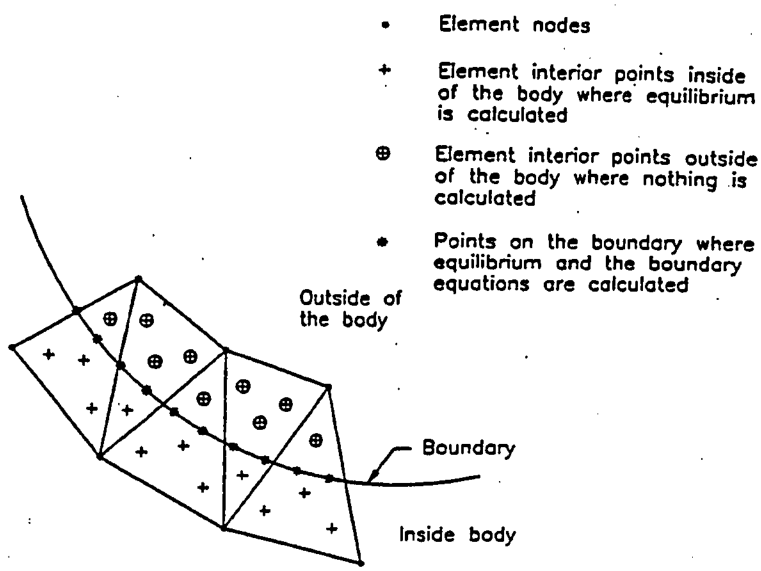

Figure 4 Plot showing which points are used in the problem solution in the optimization area.

CHAPTER 3

Fillet Problem Optimization

One of the most common examples in shape optimization is the selection of the best shape for a fillet in a plate under tension. The shape of the transition zone between the two different widths is to be optimized to minimize the stress concentration. Figure 5 shows the loads and structure that are to be analyzed. The boundary between points B_1 and B_2 is the section to be optimized. Due to symmetry only a quarter of the plate was modeled. The model shown in Figure 6 consists of 127 elements specified by 212 nodes, which give the problem 702 degrees of freedom. Boundary B_1-B_2 is divided into 120 equally space points where the equilibrium and boundary equations were calculated.

The boundary, B_1-B_2 was specified by an ellipse, shown if Figure 7, with the two design variables being the location of the center of the ellipse X_c and Y_c. In order to maintain a smooth transition between the horizontal and vertical faces, the slopes of the ellipse at the major and minor axis were forced to match the slope of the matching faces. The design variables were constrained to be in the shaded area. This effectively limits the design to the area defined in the elements. Should the design wander outside of the design space, a constraint is violated and a large error residual is added to the sum of squares, which forces the solution back into the design space.

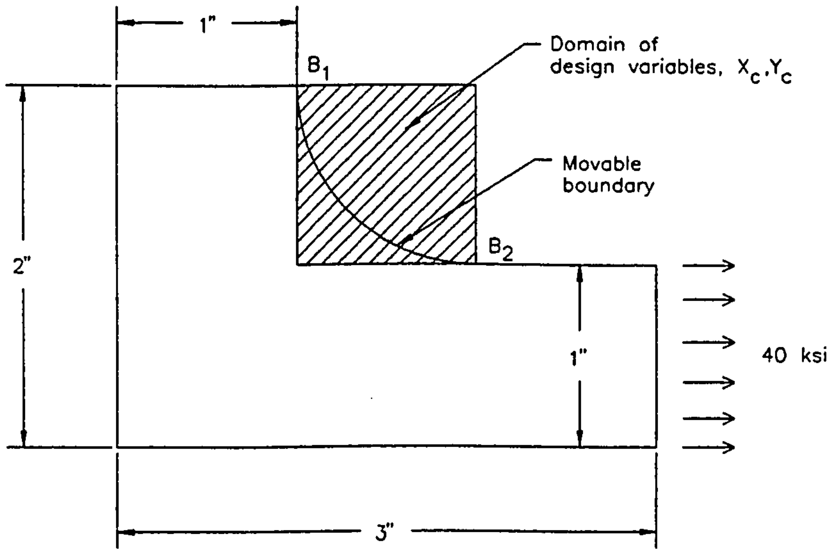

Figure 5 Fillet problem dimensions and loading.

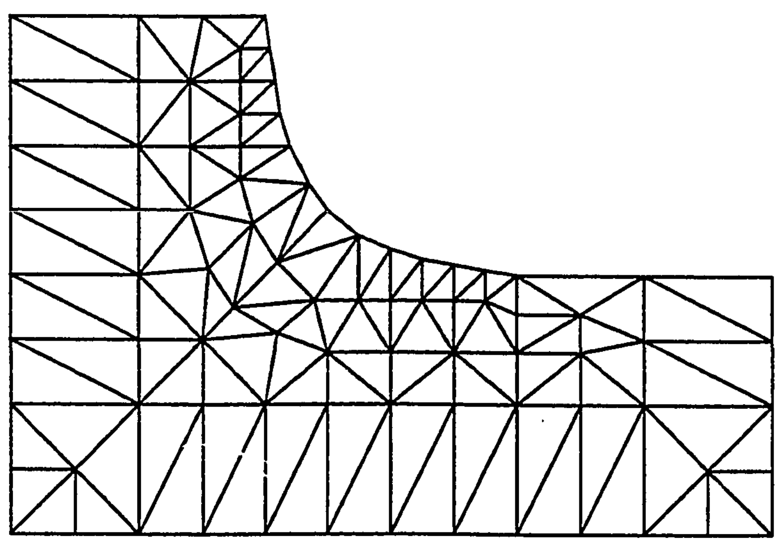

Figure 6 Element mesh used for modeling the fillet problem.

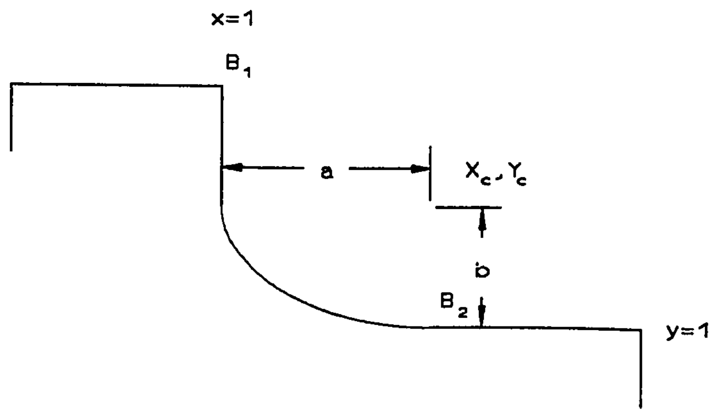

Figure 7 Diagram showing the design variables for the elliptical boundary.

In order to have a properly posed problem two boundary conditions must be specified for each boundary. For the two symmetric boundaries, $x=0$ and $y=0$, the u and v displacements, respectively, were constrained. These are nodal unknowns, so the degrees of freedom for the problem was reduced. For the remaining boundaries the normal and shear stresses were zero, except for the $x=3$ end which had an applied stress of *40 ksi*.

The objective function for the shape optimization was to minimize the area under the fillet with the constraint that the maximum stress along the surface does not exceed a yield stress of *55 ksi*. This corresponds to a stress concentration, $K_t=1.375$. Since this is the part of the problem with the highest stress gradients, the boundary residuals along the optimized section were weighted ten times more than the remaining boundaries. This forced a more accurate solution along the optimized section, without affecting the accuracy of the remaining boundaries. The interior equilibrium residuals in equation 2-7, were weighted by the area of the corresponding element multiplied by a factor of 10^5. This was required as the equilibrium residuals were on the order of 10^{-6} and the boundary residuals were around *0.1–0.5*.

Fillet Problem Results

The fillet problem was successfully solved using the new simultaneous moving boundary least squares optimization method. The final maximum stress on the boundary was *54.3 ksi* which corresponds to a K_t of *1.358*. This is just under the *55 ksi* yield strength that was the target stress. The area was reduced by *51%* from *0.54* in^2 to *0.026* in^2 The principal stress contours and the final design are shown in Figures 8,9. The rapid convergency of the solution is shown in Figure 10, which shows the number of iterations against the fillet area. In this plot iterations correspond to the iterations from Powell's method of solving for the solution vector, not design iterations. Figure 8 shows the problem converged to the final area in only *5* iterations. Solution results were verified by comparing with finite element results as shown in Figures 11,12, and Table 1, which show excellent agreement with the least squares results.

	Least Squares	Finite Element
Principal Stress σ_I	54.3	55.8
Principal Stress σ_{II}	5.5	6.7
Stress Concentration K_t	1.358	1.395

Table 1 Comparison of least squares and finite element results.

Computer Implementation

The fillet problem was solved using a computer code written in double precision Fortran. This code reads in a file containing the nodal, element, and boundary information, then assembles the elements. The differential equations are evaluated at the four interior gauss points and along the boundary using the shape functions. The residual errors are then sent to the Powell's least square subroutine which iteratively solves for the nodal unknowns. The final shape, stresses, and displacements are then printed in the output file.

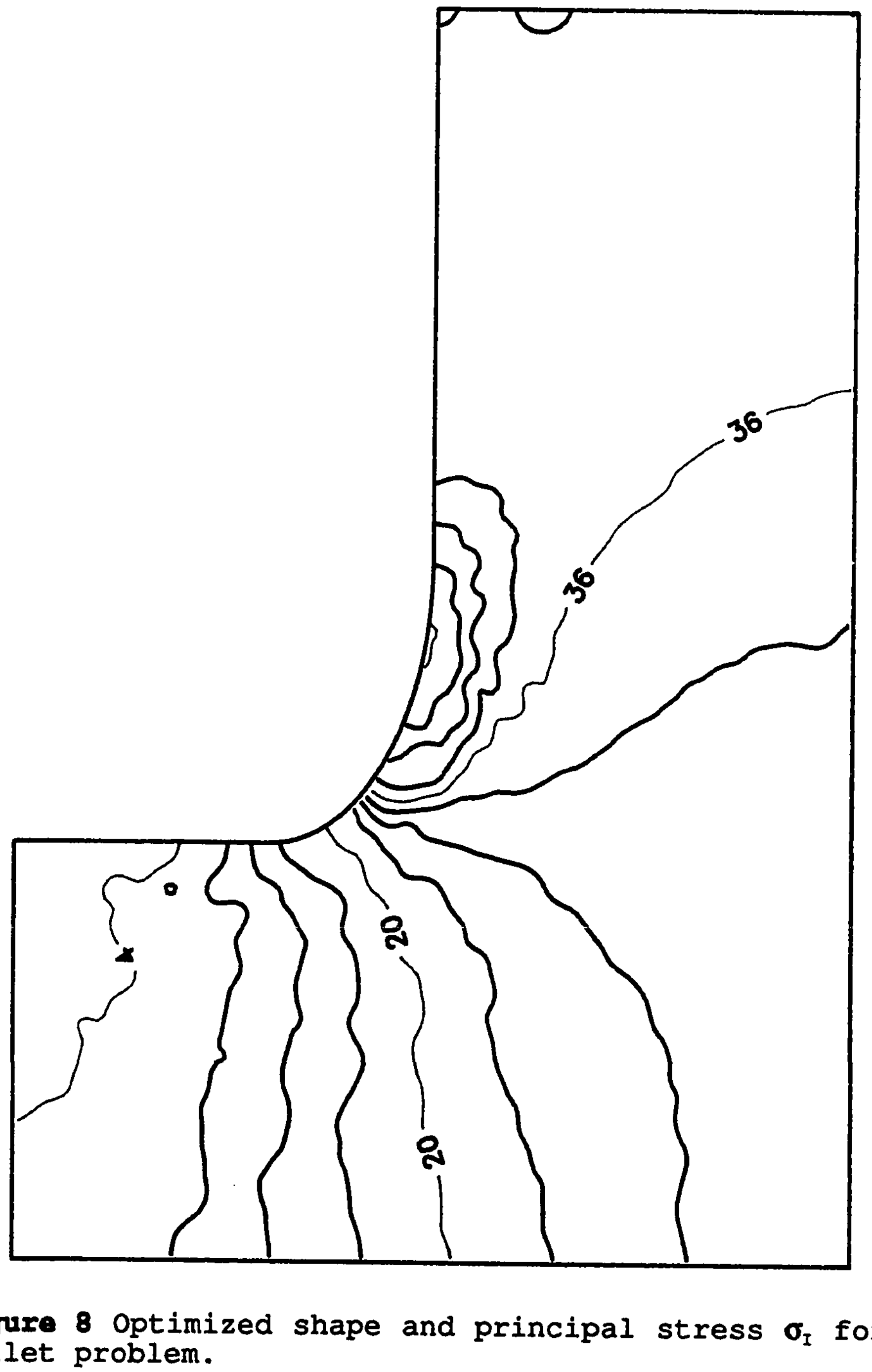

Figure 8 Optimized shape and principal stress σ_I for the fillet problem.

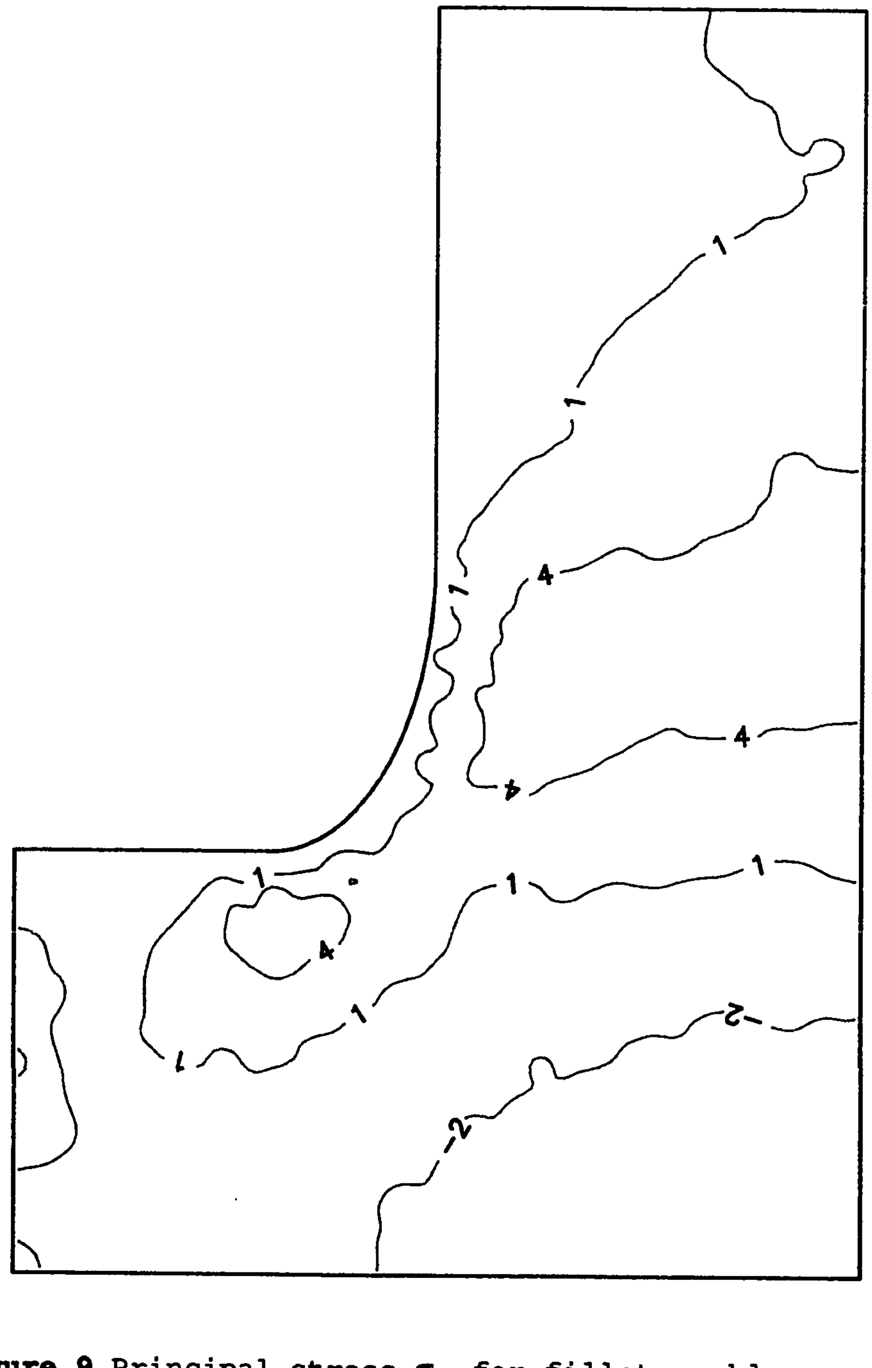

Figure 9 Principal stress σ_{II} for fillet problem.

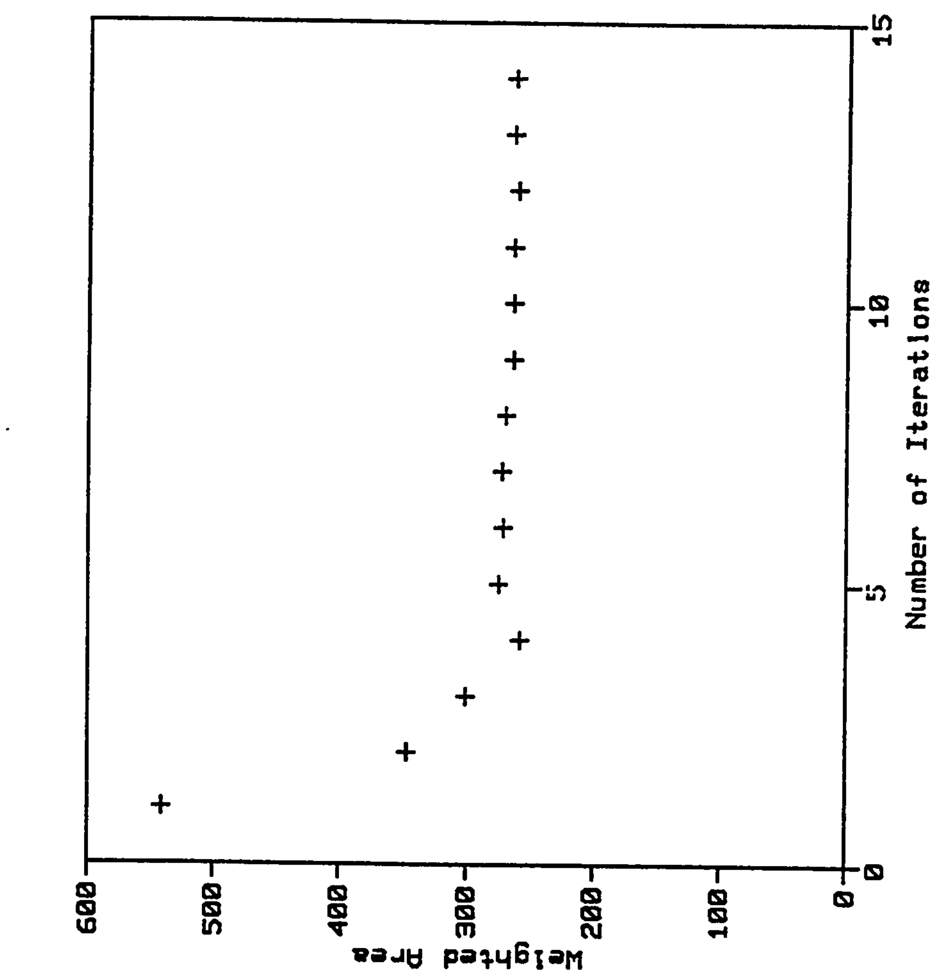

Figure 10 Plot of fillet area versus number of least squares iterations.

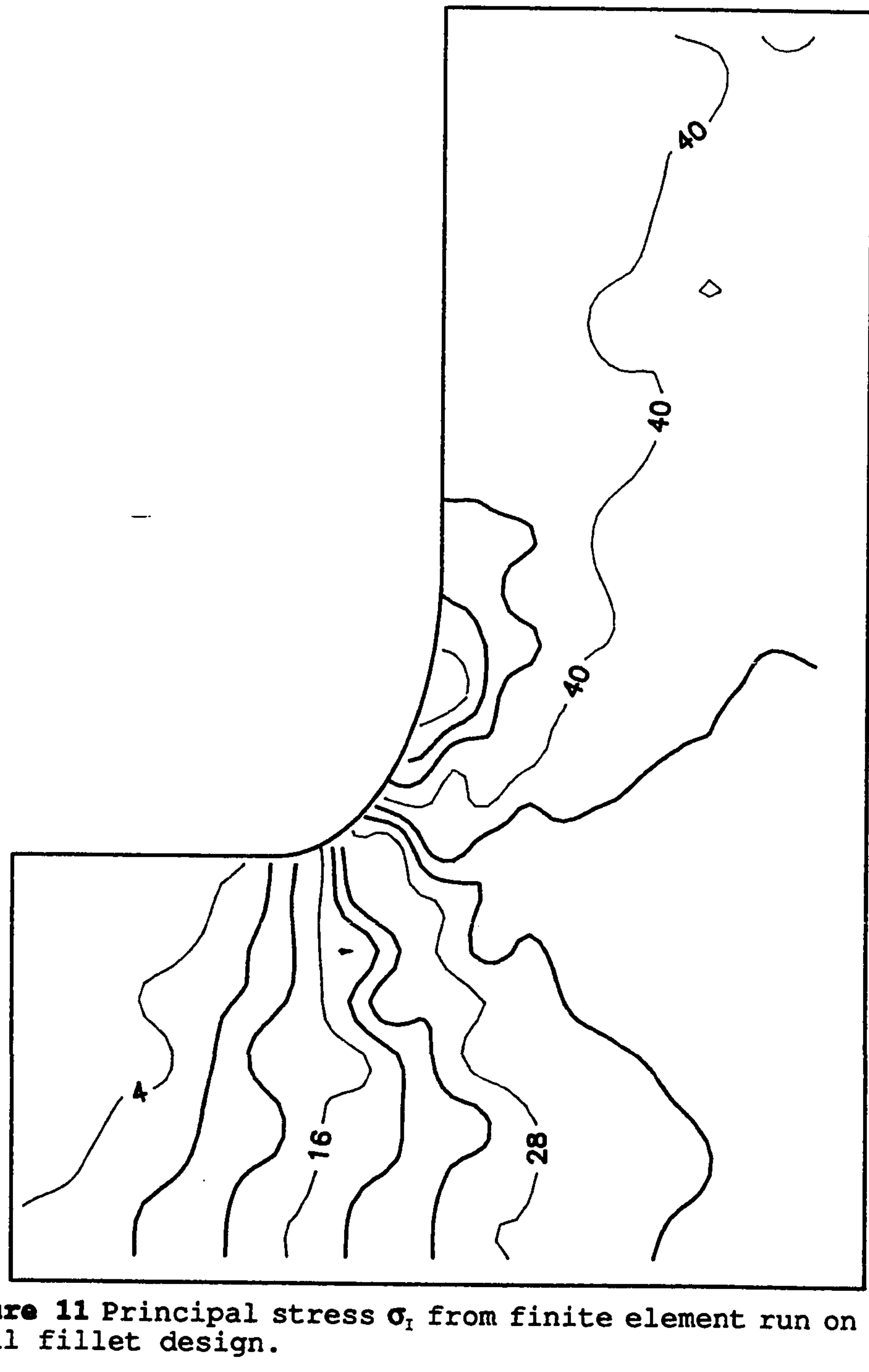

Figure 11 Principal stress σ_I from finite element run on the final fillet design.

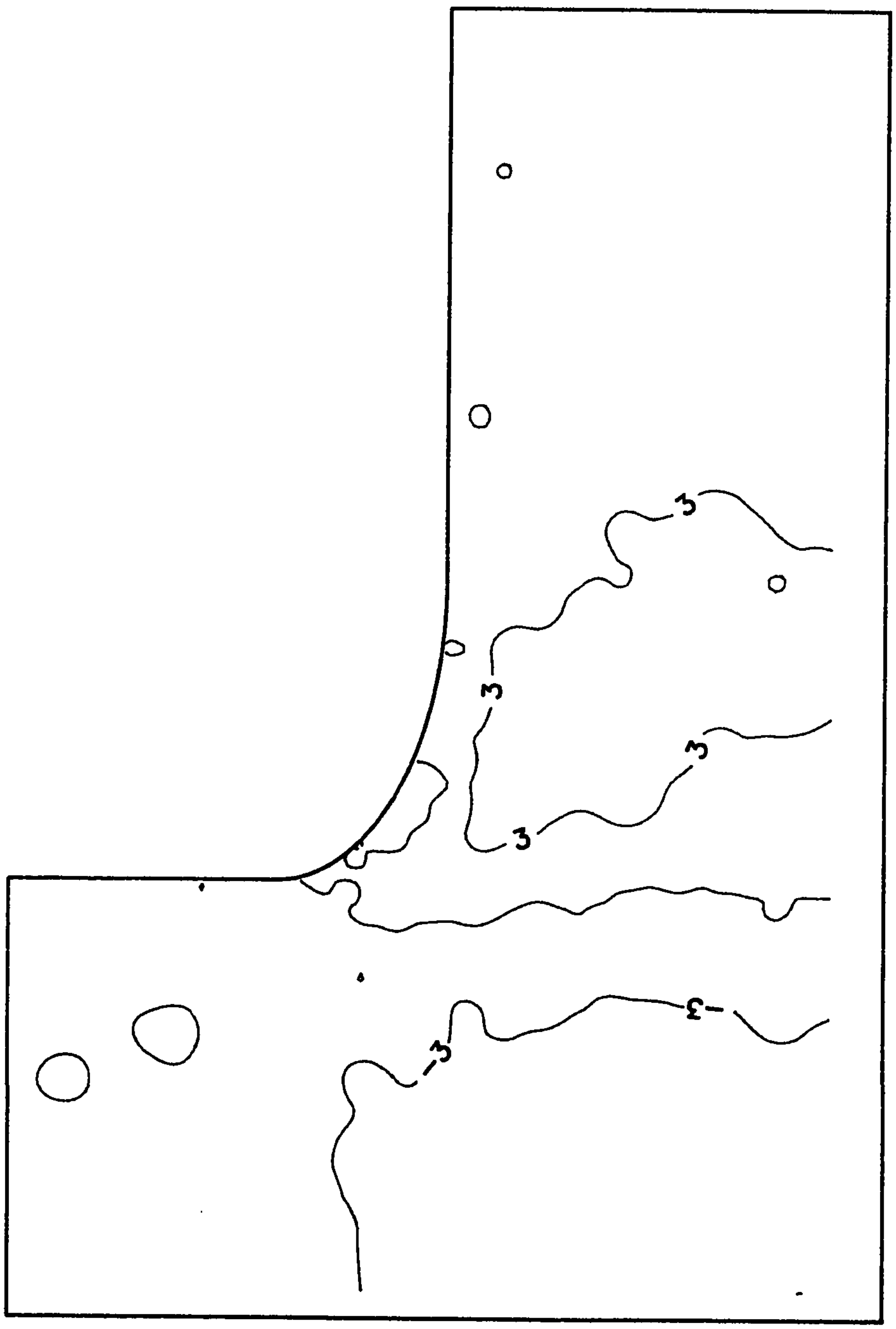

Figure 12 Principal stress σ_{II} from finite element run on the final fillet design.

Comparison with Other Solutions

The new optimization procedure will be compared with results from three different optimization methods. These methods are (1) the material derivative method, (2) the minimum compliance model with the boundary integral method, and (3) the applicatiom of higher order p-version finite elements.

The fillet problem was solved using the material derivative method with adaptive mesh refinement by Haug[20]. They used coarse (82 elements) and fine (186 elements) meshes made with constant stress triangles for the model and defined the optimized boundary by grid points connected by piecewise linear functions. The objective function was to minimize the area under the fillet such that no yielding occurs. The two models gave very similar final shapes, with the finer mesh more accurately defining the stress concentration. The fillet geometry was different from the one in this study so a direct comparison is not possible. However, their final optimized shape shown in Figure 13, is similar to the one presented in Figure 8.

The second fillet solution by Mota-Soares[21] used the boundary integral method to solve the minimum compliance problem. The boundary integral method is a weighted residual method that solves the boundary equations by the integration of approximating functions, and forcing the solution to match at the boundary. The optimization problem was to find the optimum boundary which minimizes the compliance of the structure subject to an area constraint. This method requires automatic mesh refinement around the boundary. The model consisted of 24 linear and quadratic elements, and nine design variables, which gave 76 degrees of freedom. The final shape shown in Figure 14 is very similar to the one generated by the least squares method, and gave a stress concentration factor of 1.37 compared with 1.358 from this method.

The final solution by Shyy and Fluery[12] uses high order p-version finite elements with linear mapping using Bezier and B-splines. The p-version elements are parametric elements that model both the geometry and its behavior through a coordinate transformation. These use higher order polynomials, $2 < p < 8$ for shape functions. This method accurately predicts stresses on the boundary which is important because the critical stresses in this problem are on the boundary. The derivatives for the sensitivity analysis are computed by the finite difference method. The fillet was optimized to minimize the stress concentration factor. The final stress concentration was 1.22. The final shape and stress contours are shown in Figure 15.

Table 2 shows a comparison of th K_t results from the methods.

	Least Squares	Boundary Integral	p-version F.E.
K_t	1.358	1.37	1.22

Table 2 Comparison of stress concentration factor results.

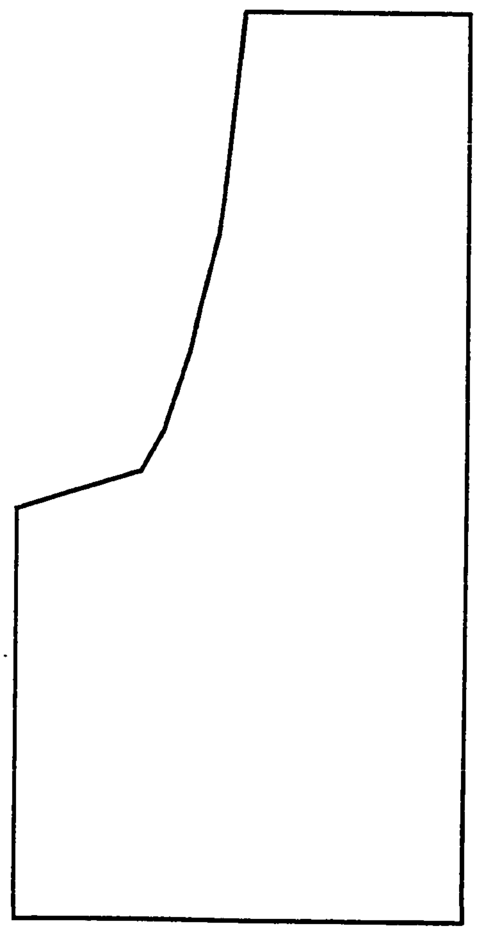

Figure 13 Optimum shape of the fillet using the Material derivative method[20].

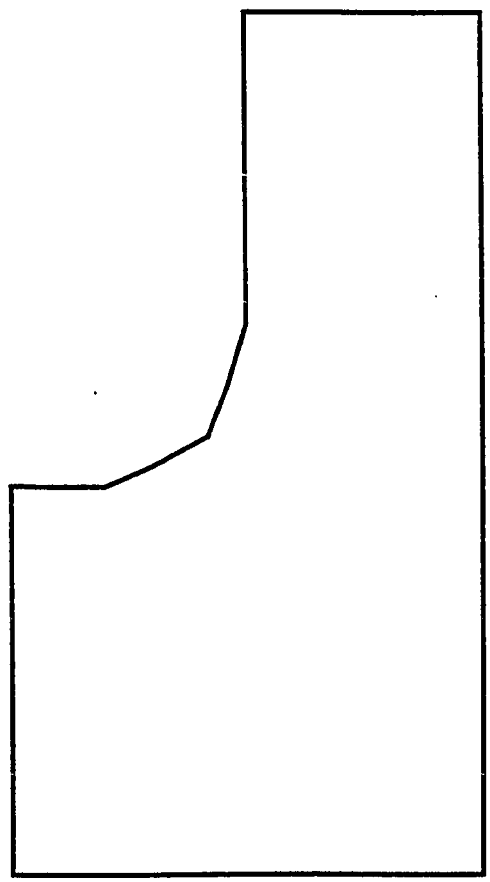

Figure 14 Optimum fillet shape using the compliance model and boundary integrals[21].

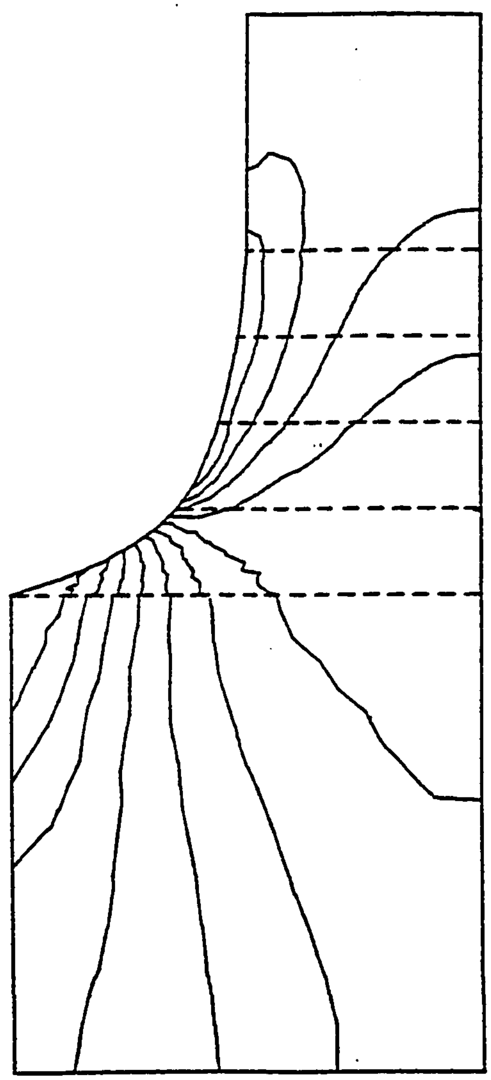

Figure 15 Optimum fillet shape using the finite element method and higher order p-elements[12].

CHAPTER 4

Conclusions

A new method for shape optimization which simultaneously solves the analysis problem and the optimum shape has been developed. The simultaneous solution is possible because the boundary no longer needs to be specified by nodes. It can move inside the elements, thereby removing any element distortion problems or remeshing requirements. This method uses the discrete least squares method to solve the governing differential equations, using a cubic finite element as the approximating function. The fillet shape optimization problem was run and the results compared to existing solutions. The new method has been shown to converge quickly to an accurate solution. The relative weighting of the interior and boundary residuals remains to be investigated as the final solution is dependent on proper weighting.

Appendix A

Computer Output for the Fillet Problem.

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C O N T R O L   P A R A M E T E R S

NUMBER OF NODAL POINTS 85

DEGREES OF FREEDOM PER NODE 2

NUMBER OF ELEMENTS 127

NUMBER OF MATERIAL SETS 1

ANALYSIS OPTION 1
  0 = PLANE STRESS
  1 = PLANE STRAIN

DATA FILE NAME mod4t.dat

N O D A L   C O O R D I N A T E   D A T A

NODE NUMBER	X1	X2
1	0.000000D+00	0.000000D+00
2	0.250000D+00	0.250000D+00
3	0.000000D+00	0.500000D+00
4	0.000000D+00	0.750000D+00
5	0.000000D+00	0.100000D+01
6	0.000000D+00	0.125000D+01
7	0.000000D+00	0.150000D+01
8	0.000000D+00	0.175000D+01
9	0.000000D+00	0.200000D+01
10	0.500000D+00	0.200000D+01
11	0.500000D+00	0.175000D+01
12	0.500000D+00	0.150000D+01
13	0.500000D+00	0.125000D+01
14	0.500000D+00	0.100000D+01
15	0.500000D+00	0.750000D+00
16	0.500000D+00	0.500000D+00
17	0.500000D+00	0.000000D+00
18	0.750000D+00	0.000000D+00
19	0.100000D+01	0.000000D+00
20	0.100000D+01	0.500000D+00
21	0.750000D+00	0.500000D+00
22	0.105000D+01	0.775000D+00
23	0.750000D+00	0.750000D+00
24	0.875000D+00	0.875000D+00
25	0.775000D+00	0.102500D+01
26	0.950000D+00	0.120000D+01
27	0.700000D+00	0.125000D+01
28	0.900000D+00	0.137500D+01
29	0.700000D+00	0.150000D+01
30	0.900000D+00	0.150000D+01
31	0.900000D+00	0.162500D+01
32	0.700000D+00	0.175000D+01
33	0.900000D+00	0.175000D+01

34	0.900000D+00	0.187500D+01
35	0.750000D+00	0.200000D+01
36	0.100000D+01	0.200000D+01
37	0.102000D+01	0.187500D+01
38	0.104000D+01	0.175000D+01
39	0.106000D+01	0.162500D+01
40	0.110000D+01	0.150000D+01
41	0.117500D+01	0.135000D+01
42	0.125000D+01	0.125000D+01
43	0.105000D+01	0.105000D+01
44	0.120000D+01	0.900000D+00
45	0.137500D+01	0.115000D+01
46	0.150000D+01	0.110000D+01
47	0.150000D+01	0.900000D+00
48	0.137500D+01	0.900000D+00
49	0.125000D+01	0.700000D+00
50	0.150000D+01	0.700000D+00
51	0.150000D+01	0.500000D+00
52	0.125000D+01	0.500000D+00
53	0.125000D+01	0.000000D+00
54	0.150000D+01	0.000000D+00
55	0.175000D+01	0.000000D+00
56	0.200000D+01	0.000000D+00
57	0.200000D+01	0.500000D+00
58	0.175000D+01	0.500000D+00
59	0.175000D+01	0.700000D+00
60	0.200000D+01	0.700000D+00
61	0.162500D+01	0.900000D+00
62	0.162500D+01	0.106000D+01
63	0.175000D+01	0.104000D+01
64	0.175000D+01	0.900000D+00
65	0.187500D+01	0.900000D+00
66	0.187500D+01	0.102000D+01
67	0.200000D+01	0.850000D+00
68	0.200000D+01	0.100000D+01
69	0.225000D+01	0.850000D+00
70	0.250000D+01	0.100000D+01
71	0.225000D+01	0.700000D+00
72	0.250000D+01	0.750000D+00
73	0.225000D+01	0.500000D+00
74	0.250000D+01	0.500000D+00
75	0.225000D+01	0.000000D+00
76	0.250000D+01	0.000000D+00
77	0.275000D+01	0.000000D+00
78	0.275000D+01	0.250000D+00
79	0.300000D+01	0.000000D+00
80	0.300000D+01	0.250000D+00
81	0.300000D+01	0.500000D+00
82	0.300000D+01	0.750000D+00
83	0.300000D+01	0.100000D+01
84	0.250000D+00	0.000000D+00
85	0.000000D+00	0.250000D+00

NODAL BOUNDARY CONDITIONS

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NODE NUMBER	DOF	VALUE
1	1	0.000000D+00
85	1	0.000000D+00
3	1	0.000000D+00
4	1	0.000000D+00
5	1	0.000000D+00
6	1	0.000000D+00
7	1	0.000000D+00
8	1	0.000000D+00
9	1	0.000000D+00
1	4	0.000000D+00
84	4	0.000000D+00
17	4	0.000000D+00
18	4	0.000000D+00
19	4	0.000000D+00
53	4	0.000000D+00
54	4	0.000000D+00
55	4	0.000000D+00
56	4	0.000000D+00
75	4	0.000000D+00
76	4	0.000000D+00
77	4	0.000000D+00
79	4	0.000000D+00
1	3	0.000000D+00
1	5	0.000000D+00
84	3	0.000000D+00
84	5	0.000000D+00
17	3	0.000000D+00
17	5	0.000000D+00
18	3	0.000000D+00
18	5	0.000000D+00
19	3	0.000000D+00
19	5	0.000000D+00
53	3	0.000000D+00
53	5	0.000000D+00
54	3	0.000000D+00
54	5	0.000000D+00
55	3	0.000000D+00
55	5	0.000000D+00
56	3	0.000000D+00
56	5	0.000000D+00
75	3	0.000000D+00
75	5	0.000000D+00
76	3	0.000000D+00
76	5	0.000000D+00
77	3	0.000000D+00
77	5	0.000000D+00
79	3	0.000000D+00
79	5	0.000000D+00
9	3	0.000000D+00
9	5	0.000000D+00
8	3	0.000000D+00
8	5	0.000000D+00
7	3	0.000000D+00
7	5	0.000000D+00
6	3	0.000000D+00

6	5	0.000000D+00
5	3	0.000000D+00
5	5	0.000000D+00
4	3	0.000000D+00
4	5	0.000000D+00
3	3	0.000000D+00
3	5	0.000000D+00
85	3	0.000000D+00
85	5	0.000000D+00

M A T E R I A L   D A T A

MATERIAL NUMBER	YOUNGS MODULUS	POISSONS RATIO	THICKNESS
1	0.300000D+05	0.300000D+00	0.100000D+01

E L E M E N T   D A T A

ELEMENT NUMBER	MATERIAL NUMBER	NODE 1	NODE 2	NODE 3
1	1	1	84	2
2	1	1	2	85
3	1	84	17	2
4	1	2	17	16
5	1	3	2	16
6	1	85	2	3
7	1	3	16	4
8	1	4	16	15
9	1	4	15	5
10	1	5	15	14
11	1	5	14	6
12	1	6	14	13
13	1	6	13	7
14	1	7	13	12
15	1	7	12	8
16	1	8	12	11
17	1	8	11	9
18	1	9	11	10
19	1	11	32	10
20	1	10	32	35
21	1	35	34	36
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23	1	32	33	34
24	1	32	31	33
25	1	29	31	32
26	1	12	29	32
27	1	12	32	11
28	1	29	30	31
29	1	29	28	30
30	1	27	28	29
31	1	12	27	29
32	1	13	27	12

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33	1	14	27	13
34	1	14	25	27
35	1	27	26	28
36	1	25	26	27
37	1	25	24	26
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39	1	15	23	14
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41	1	23	24	25
42	1	24	44	43
43	1	24	22	44
44	1	23	22	24
45	1	16	23	15
46	1	16	21	23
47	1	21	20	23
48	1	23	20	22
49	1	17	21	16
50	1	17	18	21
51	1	18	20	21
52	1	18	19	20
53	1	19	53	52
54	1	19	52	20
55	1	53	51	52
56	1	53	54	51
57	1	20	52	49
58	1	20	49	22
59	1	22	49	44
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63	1	50	61	47
64	1	49	51	50
65	1	50	59	61
66	1	61	59	64
67	1	59	65	64
68	1	59	60	65
69	1	65	67	68
70	1	65	60	67
71	1	51	59	50
72	1	51	58	59
73	1	59	57	60
74	1	58	57	59
75	1	54	58	51
76	1	54	55	58
77	1	55	57	58
78	1	55	56	57
79	1	34	37	36
80	1	33	37	34
81	1	33	38	37
82	1	31	38	33
83	1	31	39	38
84	1	30	39	31
85	1	30	40	39
86	1	28	40	30
87	1	28	41	40
88	1	26	41	28

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89	1	26	43	41
90	1	43	42	41
91	1	43	45	42
92	1	43	44	45
93	1	44	48	45
94	1	48	46	45
95	1	48	47	46
96	1	47	62	46
97	1	47	61	62
98	1	61	63	62
99	1	61	64	63
100	1	64	66	63
101	1	64	65	66
102	1	65	68	66
103	1	68	69	70
104	1	67	69	68
105	1	69	72	70
106	1	60	69	67
107	1	60	71	69
108	1	71	72	69
109	1	57	71	60
110	1	57	73	71
111	1	73	74	71
112	1	71	74	72
113	1	56	73	57
114	1	56	75	73
115	1	75	74	73
116	1	75	76	74
117	1	76	78	74
118	1	76	77	78
119	1	77	79	78
120	1	78	79	80
121	1	78	80	81
122	1	74	78	81
123	1	74	81	72
124	1	72	81	82
125	1	72	82	70
126	1	70	82	83
127	1	52	51	49

OPTIMIZATION RESULTS

X COORD	Y COORD	TANGENTIAL STRESS	NORMAL STRESS	SHEAR STRESS
1.0000	1.3883	0.150602D+02	-.905657D+00	0.114327D+01
1.0169	1.3023	0.189997D+02	0.102383D+01	0.106243D+01
1.0339	1.2674	0.201005D+02	0.555713D+00	0.111784D+01
1.0508	1.2411	0.234255D+02	0.696727D+00	0.566522D+00

1.0679	1.2195	0.247476D+02	-.213536D-01	0.219647D+00
1.0847	1.2008	0.260876D+02	-.709371D+00	-.194865D+00
1.1017	1.1842	0.274411D+02	-.137129D+01	-.648799D+00
1.1186	1.1694	0.351236D+02	0.133390D+01	0.238972D+00
1.1356	1.1559	0.375355D+02	0.368597D+00	-.187578D+00
1.1525	1.1435	0.396144D+02	-.149961D+00	-.104364D+00
1.1695	1.1320	0.414109D+02	-.339867D+00	0.183808D+00
1.1864	1.1214	0.426319D+02	-.927594D-01	0.239941D+00
1.2034	1.1116	0.433128D+02	0.579058D+00	0.206109D+00
1.2203	1.1024	0.451759D+02	-.958140D+00	0.358852D+00
1.2373	1.0938	0.459929D+02	-.759268D+00	0.267743D+00
1.2542	1.0858	0.468116D+02	-.632916D+00	0.199125D+00
1.2712	1.0783	0.476319D+02	-.574795D+00	0.153128D+00
1.2881	1.0712	0.484552D+02	-.582554D+00	0.130132D+00
1.3051	1.0646	0.492843D+02	-.655324D+00	0.130434D+00
1.3220	1.0584	0.510086D+02	0.283613D+00	-.680466D+00
1.3390	1.0526	0.514840D+02	0.291038D+00	-.836281D+00
1.3559	1.0472	0.519516D+02	0.248551D+00	-.982627D+00
1.3729	1.0421	0.524119D+02	0.157837D+00	-.111869D+01
1.3898	1.0374	0.499364D+02	-.764579D+00	-.888671D+00
1.4068	1.0329	0.503486D+02	-.569121D+00	-.580999D+00
1.4237	1.0288	0.505778D+02	-.475056D+00	-.351599D+00
1.4407	1.0250	0.506175D+02	-.472112D+00	-.188647D+00
1.4576	1.0215	0.522705D+02	0.557553D+00	-.562277D+00
1.4746	1.0183	0.522543D+02	0.666750D+00	-.636621D+00
1.4915	1.0154	0.522416D+02	0.692430D+00	-.709550D+00
1.5085	1.0127	0.499301D+02	-.232158D+00	-.646319D+00
1.5254	1.0103	0.496410D+02	-.171832D+00	-.273463D+00
1.5424	1.0082	0.492699D+02	-.130155D+00	0.188289D-01
1.5593	1.0063	0.488067D+02	-.973565D-01	0.240878D+00
1.5763	1.0047	0.482428D+02	-.652818D-01	0.403477D+00
1.5932	1.0033	0.496633D+02	0.556070D+00	0.193014D+00
1.6102	1.0021	0.490903D+02	0.390895D+00	0.282338D+00
1.6271	1.0012	0.487662D+02	0.216448D+00	-.365940D+00
1.6441	1.0006	0.480931D+02	0.202347D+00	-.282237D+00
1.6610	1.0002	0.474196D+02	0.135851D+00	-.359835D+00
1.6780	1.0000	0.467250D+02	0.383222D-01	-.597765D+00
1.6949	1.0000	0.460014D+02	-.847593D-01	-.477548D+00
1.7119	1.0000	0.452218D+02	-.213862D+00	-.406026D+00
1.7288	1.0000	0.448668D+02	0.978730D+00	-.677568D+00
1.7458	1.0000	0.441859D+02	0.573365D+00	-.416671D+00
1.7627	1.0000	0.439696D+02	0.544655D+00	-.386598D+00
1.7797	1.0000	0.432143D+02	0.353710D+00	-.170884D+00
1.7966	1.0000	0.424963D+02	0.201953D+00	-.218110D-01
1.8136	1.0000	0.418155D+02	0.893840D-01	0.606211D-01
1.8305	1.0000	0.411719D+02	0.160037D-01	0.764125D-01
1.8475	1.0000	0.405656D+02	-.181883D-01	0.255630D-01
1.8644	1.0000	0.396330D+02	0.107449D+00	0.834645D-01
1.8814	1.0000	0.389438D+02	0.620154D-01	0.120039D+00
1.8983	1.0000	0.385848D+02	0.140380D+00	0.126022D+00
1.9153	1.0000	0.382369D+02	0.189907D+00	0.117590D+00
1.9322	1.0000	0.379001D+02	0.210598D+00	0.947419D-01
1.9492	1.0000	0.375743D+02	0.202452D+00	0.574775D-01
1.9661	1.0000	0.372597D+02	0.165469D+00	0.579696D-02
1.9831	1.0000	0.369561D+02	0.996496D-01	-.602996D-01
2.0000	1.0000	0.366626D+02	0.454463D-02	-.140745D+00

1.6814	1.0000	0.465790D+02	0.165462D-01	-.666061D+00
1.4823	1.0169	0.522482D+02	0.688628D+00	-.669953D+00
1.4030	1.0339	0.502720D+02	-.603633D+00	-.642596D+00
1.3443	1.0508	0.516322D+02	0.282941D+00	-.883441D+00
1.2967	1.0678	0.488754D+02	-.611404D+00	0.127363D+00
1.2565	1.0847	0.469215D+02	-.621225D+00	0.191633D+00
1.2217	1.1017	0.452411D+02	-.939453D+00	0.350744D+00
1.1911	1.1186	0.428725D+02	0.516696D-01	0.234384D+00
1.1641	1.1356	0.409003D+02	-.326558D+00	0.124771D+00
1.1400	1.1525	0.380537D+02	0.131523D+00	-.970713D-01
1.1185	1.1695	0.351008D+02	0.134260D+01	0.247309D+00
1.0993	1.1864	0.272513D+02	-.128008D+01	-.583709D+00
1.0822	1.2034	0.258888D+02	-.609606D+00	-.130664D+00
1.0671	1.2203	0.246899D+02	0.916173D-02	0.236351D+00
1.0537	1.2373	0.236426D+02	0.576117D+00	0.515553D+00
1.0419	1.2542	0.227470D+02	0.107941D+01	0.705217D+00
1.0317	1.2712	0.199494D+02	0.632021D+00	0.110608D+01
1.0231	1.2881	0.193689D+02	0.894527D+00	0.107178D+01
1.0158	1.3051	0.189388D+02	0.104024D+01	0.106251D+01
1.0100	1.3220	0.186685D+02	0.107172D+01	0.107813D+01
1.0055	1.3390	0.185740D+02	0.983378D+00	0.112900D+01
1.0024	1.3559	0.186735D+02	0.766750D+00	0.123864D+01
1.0005	1.3729	0.147985D+02	-.107515D+01	0.121411D+01
1.0000	1.3898	0.150896D+02	-.894751D+00	0.105539D+01
1.0000	1.4068	0.151547D+02	-.506435D+00	0.341998D+00
1.0000	1.4237	0.147261D+02	0.368525D+00	0.146716D+00
1.0000	1.4407	0.118229D+02	-.151905D+00	-.371591D+00
1.0000	1.4576	0.117618D+02	0.229397D+00	-.465032D+00
1.0000	1.4746	0.117644D+02	0.709115D+00	-.555521D+00
1.0000	1.4915	0.118306D+02	0.128719D+01	-.643048D+00
1.0000	1.5085	0.548575D+01	-.839898D+00	-.596232D+00
1.0000	1.5254	0.555729D+01	-.346814D+00	-.439343D+00
1.0000	1.5424	0.564606D+01	-.468475D-02	-.331511D+00
1.0000	1.5593	0.575207D+01	0.186450D+00	-.272749D+00
1.0000	1.5763	0.587532D+01	0.226613D+00	-.263050D+00
1.0000	1.5932	0.531438D+01	0.160769D+00	-.381631D+00
1.0000	1.6102	0.544953D+01	0.468830D+00	-.362012D+00
1.0000	1.6271	0.197312D+01	-.725496D+00	-.474791D+00
1.0000	1.6441	0.226887D+01	-.389412D+00	-.218412D+00
1.0000	1.6610	0.258220D+01	-.154108D+00	-.205628D-02
1.0000	1.6780	0.271313D+01	-.195632D-01	0.174292D+00
1.0000	1.6949	0.326169D+01	0.142220D-01	0.310641D+00
1.0000	1.7119	0.362783D+01	-.527562D-01	0.406973D+00
1.0000	1.7288	0.168952D+01	-.397992D-01	-.111148D+00
1.0000	1.7458	0.234317D+01	0.404451D+00	-.269734D+00
1.0000	1.7627	-.365684D+00	-.438951D+00	-.432274D-01
1.0000	1.7797	0.964619D-01	-.258855D-01	0.188373D-01
1.0000	1.7966	0.489726D+00	0.207277D+00	0.724976D-01
1.0000	1.8136	0.814065D+00	0.260511D+00	0.117747D+00
1.0000	1.8305	0.106951D+01	0.133822D+00	0.154592D+00
1.0000	1.8475	0.125605D+01	-.172776D+00	0.183026D+00
1.0000	1.8644	0.101555D+01	0.252793D+00	-.518454D-01
1.0000	1.8814	0.795972D+00	-.250519D+00	-.894664D-01
1.0000	1.8983	0.905842D+00	-.621700D-01	-.414395D+00
1.0000	1.9153	0.930459D+00	0.591638D-01	-.589434D+00
1.0000	1.9322	0.869827D+00	0.113497D+00	-.614603D+00

1.0000	1.9492	0.723953D+00	0.100822D+00	-.489899D+00
1.0000	1.9661	0.492819D+00	0.211387D-01	-.215309D+00
1.0000	1.9831	0.176452D+00	-.125544D+00	0.209136D+00
1.0000	2.0000	-.225158D+00	-.339230D+00	0.783449D+00

FINAL AREA FROM MINIMIZATION = 2.1145891710611

X	Y	(ELIPSE CENTER)
1.6814	1.3883	
1.6814	1.3883	

S O L U T I O N   D A T A

NUMBER OF UNKNOWNS 764

NUMBER OF EQUATIONS 2077

NUMBER OF ITERATIONS 608

NUMBER OF CALFUN CALLS 10000

SUM OF SQUARES . . . . 0.299625D+05

RMS RESIDUAL . . . . 0.379814D+01

N O D A L   V A L U E S

NODE	X	Y	SIGXX	SIGYY	SIGXY	X DISP	Y DISP
1	0.000	0.000	29.551	-4.042	0.000	0.00000D+00	0.00000D+00
2	0.250	0.250	29.157	-3.627	-0.172	0.23295D-03	-.12358D-03
3	0.000	0.500	27.271	-3.860	0.000	0.00000D+00	-.24771D-03
4	0.000	0.750	24.043	-3.209	0.000	0.00000D+00	-.35852D-03
5	0.000	1.000	19.796	-2.459	0.000	0.00000D+00	-.45204D-03
6	0.000	1.250	14.424	-1.652	0.000	0.00000D+00	-.52372D-03
7	0.000	1.500	8.900	-1.050	0.000	0.00000D+00	-.57176D-03
8	0.000	1.750	2.245	-0.230	0.000	0.00000D+00	-.59430D-03
9	0.000	2.000	1.202	0.561	0.000	0.00000D+00	-.58888D-03
10	0.500	2.000	2.451	-0.133	0.153	-.88569D-04	-.49243D-03
11	0.500	1.750	0.378	0.579	-0.434	0.22729D-04	-.50507D-03
12	0.500	1.500	7.281	0.959	-0.819	0.12734D-03	-.49785D-03
13	0.500	1.250	14.061	0.460	-1.796	0.22520D-03	-.46908D-03
14	0.500	1.000	20.549	-0.717	-2.110	0.31708D-03	-.41215D-03
15	0.500	0.750	25.167	-1.774	-1.363	0.38894D-03	-.32760D-03
16	0.500	0.500	27.854	-2.107	-0.758	0.43760D-03	-.22629D-03
17	0.500	0.000	29.969	-2.537	0.000	0.47335D-03	0.00000D+00
18	0.750	0.000	30.087	-0.475	0.000	0.70606D-03	0.00000D+00

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19	1.000	0.000	30.215	1.914	0.000	0.93234D-03	0.00000D+00
20	1.000	0.500	29.651	2.265	-1.251	0.87380D-03	-.16399D-03
21	0.750	0.500	28.633	-0.345	-1.064	0.65578D-03	-.19972D-03
22	1.050	0.775	29.703	3.546	-3.286	0.82116D-03	-.23722D-03
23	0.750	0.750	26.176	-0.072	-2.032	0.58620D-03	-.29094D-03
24	0.875	0.875	25.212	1.712	-3.516	0.62803D-03	-.30466D-03
25	0.775	1.025	20.548	2.649	-4.252	0.47410D-03	-.36229D-03
26	0.950	1.200	13.431	11.042	-7.227	0.41849D-03	-.32006D-03
27	0.700	1.250	12.924	3.613	-2.666	0.30276D-03	-.41126D-03
28	0.900	1.375	7.017	11.559	0.542	0.26843D-03	-.30258D-03
29	0.700	1.500	6.628	3.655	-0.431	0.16430D-03	-.41444D-03
30	0.900	1.500	3.955	9.380	2.259	0.18189D-03	-.27217D-03
31	0.900	1.625	1.782	5.581	4.844	0.96387D-04	-.24756D-03
32	0.700	1.750	0.172	2.649	0.693	0.20663D-04	-.40019D-03
33	0.900	1.750	1.581	1.475	3.889	0.17074D-04	-.23735D-03
34	0.900	1.875	1.064	-0.231	2.265	-.66275D-04	-.23600D-03
35	0.750	2.000	0.025	-0.120	-0.012	-.13890D-03	-.34972D-03
36	1.000	2.000	0.339	-0.225	-0.783	-.16136D-03	-.15341D-03
37	1.020	1.875	1.009	1.577	-0.236	-.67112D-04	-.14140D-03
38	1.040	1.750	0.096	2.780	-1.264	0.16956D-04	-.13703D-03
39	1.060	1.625	1.764	1.755	0.503	0.90431D-04	-.13207D-03
40	1.100	1.500	5.537	12.289	0.966	0.16802D-03	-.12209D-03
41	1.175	1.350	5.004	22.573	-16.765	0.22358D-03	-.19924D-03
42	1.250	1.250	25.935	17.699	-35.741	0.41065D-03	-.30484D-03
43	1.050	1.050	24.044	6.616	-9.388	0.61925D-03	-.29792D-03
44	1.200	0.900	33.784	6.365	-6.869	0.87773D-03	-.24108D-03
45	1.375	1.150	56.289	2.826	-26.447	0.79868D-03	-.34952D-03
46	1.500	1.100	62.286	-2.775	-13.353	0.10935D-02	-.36256D-03
47	1.500	0.900	40.997	5.019	-6.249	0.11958D-02	-.24579D-03
48	1.375	0.900	38.391	6.302	-7.423	0.10541D-02	-.23368D-03
49	1.250	0.700	32.077	5.508	-3.236	0.10302D-02	-.18590D-03
50	1.500	0.700	34.763	5.468	-4.144	0.12654D-02	-.18245D-03
51	1.500	0.500	32.689	5.335	-2.941	0.13172D-02	-.12819D-03
52	1.250	0.500	31.112	4.544	-2.069	0.10924D-02	-.13431D-03
53	1.250	0.000	30.599	4.414	0.000	0.11523D-02	0.00000D+00
54	1.500	0.000	31.667	5.342	0.000	0.13723D-02	0.00000D+00
55	1.750	0.000	33.121	5.180	0.000	0.16009D-02	0.00000D+00
56	2.000	0.000	35.022	3.725	0.000	0.18451D-02	0.00000D+00
57	2.000	0.500	36.302	2.512	-3.245	0.18127D-02	-.18110D-03
58	1.750	0.500	34.583	4.379	-3.344	0.15557D-02	-.14613D-03
59	1.750	0.700	36.377	4.510	-4.016	0.15196D-02	-.21111D-03
60	2.000	0.700	37.461	1.273	-3.353	0.17923D-02	-.26518D-03
61	1.625	0.900	42.088	4.244	-3.596	0.13469D-02	-.26293D-03
62	1.625	1.060	55.132	-3.037	-0.582	0.13373D-02	-.35612D-03
63	1.750	1.040	45.172	-0.013	1.668	0.15237D-02	-.36439D-03
64	1.750	0.900	41.281	2.202	-3.082	0.14999D-02	-.28995D-03
65	1.875	0.900	39.234	0.881	-1.961	0.16500D-02	-.32587D-03
66	1.875	1.020	38.979	0.035	0.710	0.16745D-02	-.38598D-03
67	2.000	0.850	37.908	0.590	-2.035	0.17903D-02	-.33526D-03
68	2.000	1.000	36.663	0.005	-0.141	0.18119D-02	-.40743D-03
69	2.250	0.850	37.326	0.005	-1.158	0.20744D-02	-.38024D-03
70	2.500	1.000	35.071	-0.657	-0.761	0.23538D-02	-.47803D-03
71	2.250	0.700	37.572	0.483	-1.888	0.20746D-02	-.30835D-03
72	2.500	0.750	36.447	0.095	-1.023	0.23534D-02	-.35749D-03
73	2.250	0.500	37.226	1.276	-2.272	0.20859D-02	-.21658D-03
74	2.500	0.500	37.705	0.449	-1.365	0.23679D-02	-.23782D-03

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75	2.250	0.000	37.103	1.600	0.000	0.21102D-02	0.00000D+00
76	2.500	0.000	38.573	0.823	0.000	0.23936D-02	0.00000D+00
77	2.750	0.000	39.471	1.148	0.000	0.26869D-02	0.00000D+00
78	2.750	0.250	39.172	0.888	-0.632	0.26774D-02	-.11991D-03
79	3.000	0.000	39.858	3.165	0.000	0.29816D-02	0.00000D+00
80	3.000	0.250	39.839	1.871	0.196	0.29731D-02	-.10926D-03
81	3.000	0.500	39.781	0.033	-0.530	0.29507D-02	-.23157D-03
82	3.000	0.750	40.264	-0.285	-0.452	0.29345D-02	-.36117D-03
83	3.000	1.000	40.276	0.173	0.061	0.29335D-02	-.49039D-03
84	0.250	0.000	29.645	-3.662	0.000	0.23705D-03	0.00000D+00
85	0.000	0.250	28.988	-3.986	0.000	0.00000D+00	-.12599D-03

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